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Toward Correlating Structure and Function in Proteins: A LITR-XAS Study of the Photodissociation of Carbonmonoxymyoglobin

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A large portion of protein research has involved the use of ultrafast spectroscopic techniques to determine the correlation between structure and function in the photodissociation of carbonmonoxymyoglobin (MbCO), using this system as a model for protein dynamics as a whole. Accomplishing this goal requires the use of techniques with sufficient spatial resolution to measure the minute motions in the protein metal center associated with photoexcitation. Preliminary laser-initiated time-resolved x-ray absorption spectroscopy (LITR-XAS) experiments have been performed to determine the structural changes that occur in the iron heme center of MbCO upon photoexcitation. These experiments show a shift in Fe K-edge energy and the loss of a pre-edge peak, indicative of the loss of CO and motion of the Fe out of the heme plane. These results mark the first successful use of ultrafast XAS experiments to probe the structural dynamics of a protein sample, serving as a template for future studies on other proteins. Future experiments will focus on quantifying the structural changes in the protein and comparing with those in free heme to determine the effect that the protein matrix has on the photoexcited dynamics.

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